Full wwPDB X-ray Structure Validation Report (i)

Apr 27, 2024 – 11:01 am BST

PDB ID	:	2C0M
Title	:	apo form of the TPR domain of the pex5p receptor
Authors	:	Stanley, W.A.; Kursula, P.; Wilmanns, M.
Deposited on	:	2005-09-05
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

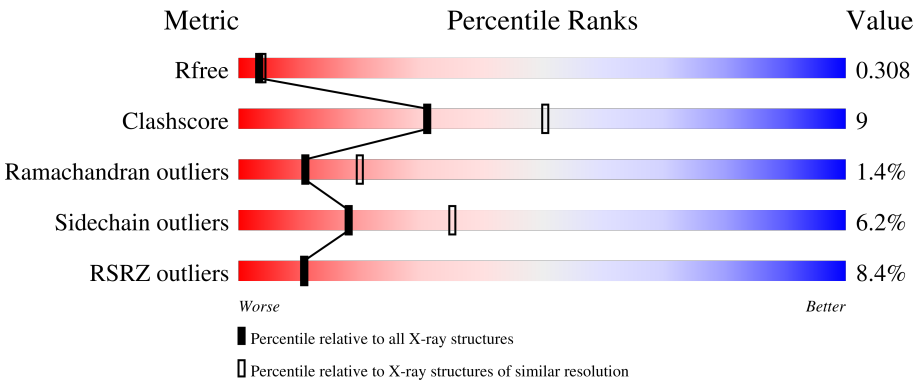
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

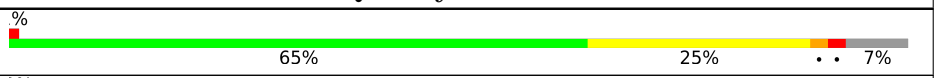
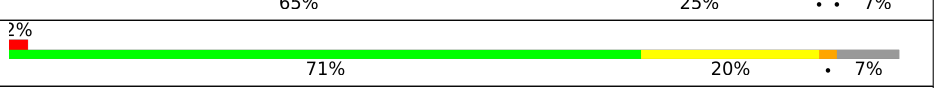
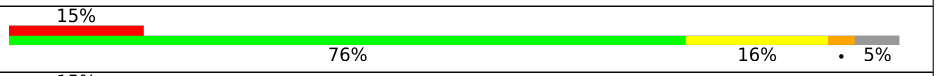
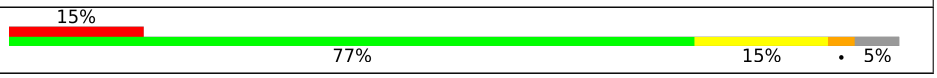
The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	319	
1	B	319	
1	C	319	
1	F	319	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9629 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PEROXISOMAL TARGETING SIGNAL 1 RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	297	2364	1482	418	453	11	0	3	0
1	B	297	2374	1489	419	455	11	0	4	0
1	C	302	2377	1493	417	456	11	0	1	0
1	F	302	2368	1488	416	453	11	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	388	ILE	THR	conflict	UNP P50542
B	388	ILE	THR	conflict	UNP P50542
C	388	ILE	THR	conflict	UNP P50542
F	388	ILE	THR	conflict	UNP P50542

- Molecule 2 is water.

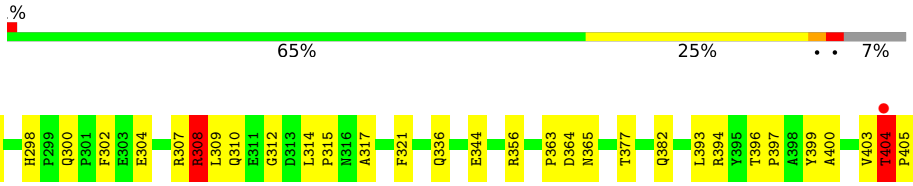
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	54	54	54	0	0
2	B	57	57	57	0	0
2	C	14	14	14	0	0
2	F	21	21	21	0	0

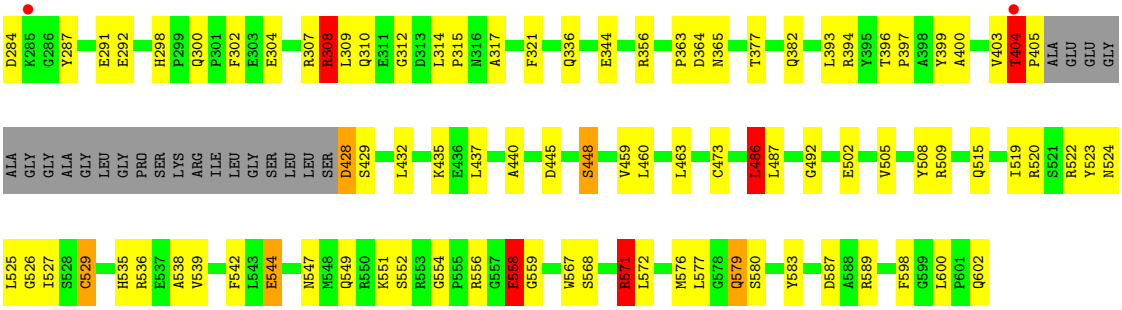
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: PEROXISOMAL TARGETING SIGNAL 1 RECEPTOR

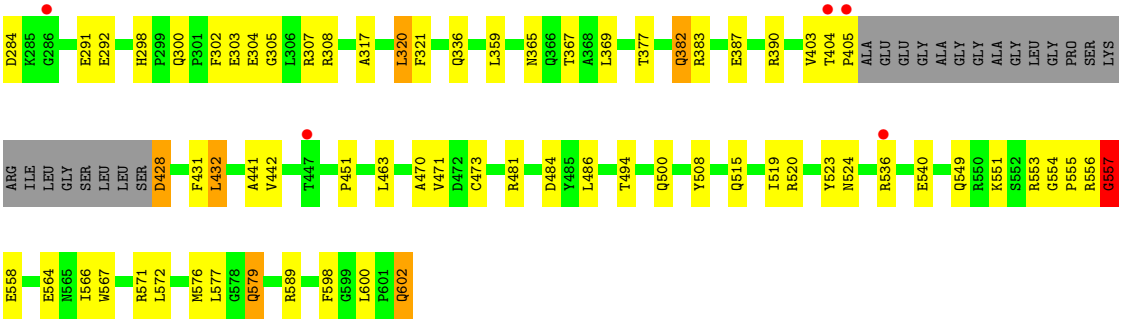
Chain A:





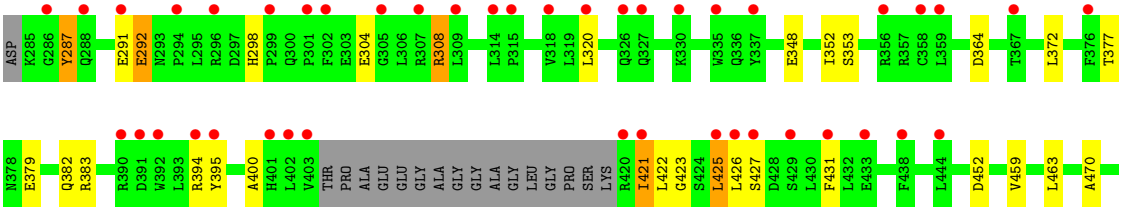
• Molecule 1: PEROXISOMAL TARGETING SIGNAL 1 RECEPTOR

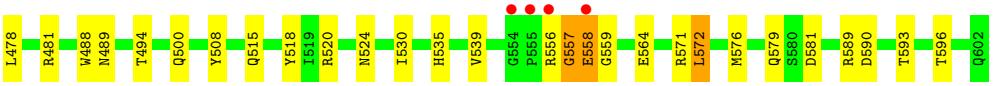
Chain B:



• Molecule 1: PEROXISOMAL TARGETING SIGNAL 1 RECEPTOR

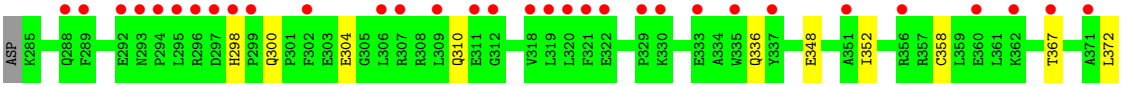
Chain C:

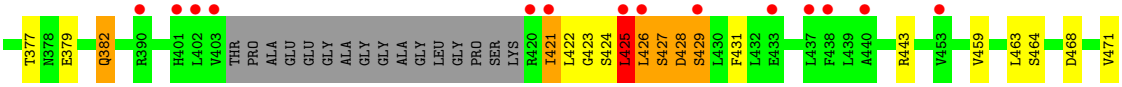


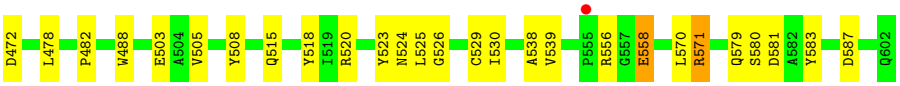


- Molecule 1: PEROXISOMAL TARGETING SIGNAL 1 RECEPTOR

Chain F:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	53.47Å 85.55Å 88.89Å 71.17° 89.99° 73.43°	Depositor
Resolution (Å)	19.54 – 2.50 19.53 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.5 (19.54-2.50) 89.6 (19.53-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.263 , 0.309 0.296 , 0.308	Depositor DCC
R_{free} test set	2363 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	27.9	Xtriage
Anisotropy	0.782	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , -1.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.229 for h,h-k,-l	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	9629	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.75% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.86	3/2409 (0.1%)	0.85	6/3265 (0.2%)
1	B	0.69	1/2419 (0.0%)	0.73	1/3278 (0.0%)
1	C	0.50	0/2421	0.62	0/3280
1	F	0.51	1/2412 (0.0%)	0.66	1/3268 (0.0%)
All	All	0.66	5/9661 (0.1%)	0.72	8/13091 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	473	CYS	CB-SG	-6.50	1.71	1.82
1	A	544	GLU	CG-CD	6.45	1.61	1.51
1	A	529	CYS	CB-SG	-6.00	1.72	1.82
1	A	473	CYS	CB-SG	-5.80	1.72	1.81
1	F	529	CYS	CB-SG	-5.15	1.73	1.81

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	308	ARG	NE-CZ-NH1	9.72	125.16	120.30
1	A	308	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	A	486	LEU	CA-CB-CG	5.67	128.34	115.30
1	F	429	SER	N-CA-CB	-5.60	102.10	110.50
1	A	308	ARG	CG-CD-NE	5.38	123.10	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	557	GLY	N-CA-C	-5.37	99.67	113.10
1	A	308	ARG	CD-NE-CZ	5.27	130.97	123.60
1	A	571	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	557	GLY	Peptide
1	C	425	LEU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2364	0	2312	64	0
1	B	2374	0	2321	47	0
1	C	2377	0	2327	29	0
1	F	2368	0	2322	33	0
2	A	54	0	0	4	0
2	B	57	0	0	0	0
2	C	14	0	0	2	0
2	F	21	0	0	1	0
All	All	9629	0	9282	171	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (171) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:426:LEU:CD1	1:F:427:SER:H	1.59	1.13
1:F:426:LEU:HD13	1:F:427:SER:H	1.35	0.91
1:F:426:LEU:HD12	1:F:427:SER:H	1.37	0.90
1:C:572:LEU:HD22	1:C:576:MET:HE3	1.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:426:LEU:CD1	1:F:427:SER:N	2.41	0.82
1:A:519:ILE:HG21	1:A:549:GLN:HE21	1.47	0.80
1:F:426:LEU:HD12	1:F:427:SER:N	1.98	0.78
1:B:536[B]:ARG:NH1	1:B:540:GLU:OE2	2.17	0.78
1:B:304:GLU:HB3	1:B:320:LEU:HD21	1.66	0.77
1:C:572:LEU:HD22	1:C:576:MET:CE	2.18	0.74
1:A:526:GLY:HA3	1:A:542:PHE:CE2	2.23	0.72
1:F:425:LEU:HD23	1:F:425:LEU:H	1.58	0.69
1:A:508:TYR:CZ	1:A:524:ASN:HB3	2.29	0.67
1:A:377[A]:THR:HG23	1:A:463:LEU:HD21	1.77	0.66
1:B:305:GLY:N	1:B:320:LEU:HD23	2.11	0.66
1:A:428:ASP:OD1	1:A:428:ASP:C	2.34	0.66
1:B:536[B]:ARG:CG	1:B:536[B]:ARG:HH11	2.08	0.66
1:A:505:VAL:HG13	1:A:525:LEU:HD11	1.79	0.65
1:A:403:VAL:HG12	1:A:405:PRO:HD2	1.79	0.65
1:A:551:LYS:NZ	1:A:602:GLN:OXT	2.30	0.64
1:A:547:ASN:ND2	1:A:602:GLN:OXT	2.30	0.64
1:C:581:ASP:OD2	1:C:581:ASP:N	2.32	0.63
1:B:508:TYR:CZ	1:B:524:ASN:HB3	2.34	0.63
1:F:377:THR:CG2	2:F:2004:HOH:O	2.48	0.62
1:B:359:LEU:HD21	1:B:369:LEU:HD12	1.82	0.61
1:C:556:ARG:O	1:C:558:GLU:N	2.34	0.60
1:A:572:LEU:HD23	1:A:576:MET:HE3	1.84	0.59
1:B:304:GLU:HB3	1:B:320:LEU:CD2	2.33	0.59
1:F:377:THR:HG23	1:F:463:LEU:HD21	1.85	0.58
1:A:308:ARG:HG3	1:A:308:ARG:HH11	1.68	0.58
1:A:519:ILE:HG21	1:A:549:GLN:NE2	2.17	0.58
1:C:557:GLY:O	1:C:559:GLY:N	2.37	0.57
1:B:298:HIS:CE1	1:B:304:GLU:HG3	2.39	0.57
1:A:298:HIS:CE1	1:A:304:GLU:HG3	2.39	0.57
1:A:428:ASP:O	1:A:432:LEU:HB2	2.04	0.57
1:B:572:LEU:HD23	1:B:576:MET:HE1	1.86	0.56
1:C:508:TYR:CZ	1:C:524:ASN:HB3	2.41	0.56
1:A:382:GLN:NE2	1:A:463:LEU:HD22	2.21	0.56
1:A:508:TYR:CE2	1:A:524:ASN:HB3	2.40	0.56
1:A:572:LEU:HD23	1:A:576:MET:CE	2.36	0.56
1:A:344:GLU:HG3	2:A:2033:HOH:O	2.04	0.56
1:A:363:PRO:HD3	2:A:2016:HOH:O	2.04	0.56
1:C:564:GLU:OE2	1:C:589:ARG:NH2	2.39	0.56
1:A:535:HIS:O	1:A:539:VAL:HG23	2.06	0.56
1:A:522:ARG:HD3	1:A:544:GLU:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:VAL:HG13	1:A:525:LEU:CD1	2.37	0.55
1:B:428:ASP:OD1	1:B:428:ASP:N	2.41	0.54
1:B:536[B]:ARG:HH11	1:B:536[B]:ARG:HG3	1.73	0.54
1:F:580:SER:HA	1:F:583:TYR:CE1	2.42	0.54
1:F:377:THR:HG21	1:F:459:VAL:HG13	1.91	0.53
1:A:508:TYR:CE1	1:A:524:ASN:HB3	2.43	0.53
1:B:553:ARG:HB3	1:B:558:GLU:HG2	1.91	0.53
1:A:486:LEU:HD12	1:A:487:LEU:HD23	1.90	0.52
1:F:382:GLN:CD	1:F:463:LEU:HD22	2.29	0.52
1:B:554:GLY:O	1:B:556:ARG:N	2.42	0.52
1:C:348:GLU:HG2	1:C:379:GLU:HG2	1.92	0.52
1:A:567:TRP:CE2	1:A:589:ARG:HG3	2.44	0.52
1:B:382:GLN:HA	1:B:382:GLN:OE1	2.08	0.52
1:B:382:GLN:OE1	1:B:382:GLN:CA	2.57	0.52
1:A:309:LEU:O	1:A:312:GLY:N	2.35	0.52
1:B:359:LEU:CD2	1:B:369:LEU:HD12	2.40	0.51
1:B:390:ARG:HH22	1:B:405:PRO:HD3	1.74	0.51
1:A:526:GLY:O	1:A:529:CYS:HB2	2.11	0.51
1:B:390:ARG:HH22	1:B:405:PRO:CD	2.24	0.51
1:B:555:PRO:C	1:B:557:GLY:H	2.13	0.51
1:A:364:ASP:OD2	1:A:364:ASP:N	2.38	0.51
1:A:377[B]:THR:HG21	1:A:459:VAL:CG1	2.40	0.51
1:A:393:LEU:CD2	1:A:437:LEU:HB3	2.42	0.49
1:B:523:TYR:CD1	1:B:566:ILE:HG12	2.46	0.49
1:A:523:TYR:CZ	1:A:527:ILE:HD11	2.47	0.49
1:F:298:HIS:CE1	1:F:304:GLU:HG3	2.47	0.49
1:A:336:GLN:NE2	1:A:365:ASN:HD21	2.10	0.49
1:F:426:LEU:HD12	1:F:427:SER:CA	2.42	0.49
1:A:508:TYR:O	1:A:509:ARG:C	2.49	0.49
1:A:529:CYS:HB3	1:A:538:ALA:HB2	1.94	0.49
1:B:336:GLN:HE21	1:B:365:ASN:HD21	1.60	0.49
1:C:382:GLN:CD	1:C:463:LEU:HD22	2.32	0.49
1:F:571:ARG:HD2	1:F:587:ASP:OD1	2.12	0.49
1:B:519:ILE:HG21	1:B:549:GLN:HE21	1.77	0.48
1:B:577:LEU:HD23	1:B:579:GLN:HB2	1.95	0.48
1:C:425:LEU:HB2	1:C:426:LEU:HD23	1.95	0.48
1:B:300:GLN:HE22	1:B:302:PHE:HB3	1.78	0.48
1:C:287:TYR:N	1:C:353:SER:OG	2.26	0.48
1:A:577:LEU:HD23	1:A:579:GLN:HB2	1.96	0.48
1:C:292:GLU:O	1:C:292:GLU:HG3	2.13	0.48
1:A:554:GLY:HA3	1:A:558:GLU:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:ARG:NH1	1:B:387:GLU:OE2	2.46	0.47
1:A:394:ARG:HA	1:A:400:ALA:HA	1.95	0.47
1:A:571:ARG:HD2	1:A:587:ASP:OD1	2.15	0.47
1:C:596:THR:HG21	1:F:482:PRO:HB3	1.96	0.47
1:A:522:ARG:O	1:A:525:LEU:HB3	2.13	0.47
1:B:564:GLU:OE2	1:B:589:ARG:NH2	2.47	0.47
1:A:284:ASP:HB2	1:A:356:ARG:NE	2.29	0.47
1:A:403:VAL:HG12	1:A:405:PRO:CD	2.44	0.46
1:F:508:TYR:CZ	1:F:524:ASN:HB3	2.50	0.46
1:F:580:SER:HA	1:F:583:TYR:CD1	2.51	0.46
1:B:377:THR:HG23	1:B:463[A]:LEU:HD21	1.98	0.46
1:B:471:VAL:HG23	1:B:494:THR:HG22	1.97	0.46
1:A:580:SER:HA	1:A:583:TYR:CE1	2.51	0.46
1:F:471:VAL:O	1:F:472:ASP:C	2.54	0.46
1:F:352:ILE:HG23	1:F:372:LEU:HD11	1.99	0.45
1:A:492:GLY:HA3	1:A:508:TYR:CE2	2.51	0.45
1:A:536[B]:ARG:CZ	1:A:598:PHE:HD2	2.30	0.45
1:B:305:GLY:CA	1:B:320:LEU:HD23	2.46	0.45
1:B:463[B]:LEU:C	1:B:463[B]:LEU:HD12	2.37	0.45
1:B:523:TYR:CE1	1:B:566:ILE:HG12	2.51	0.45
1:A:287:TYR:C	1:A:287:TYR:CD2	2.90	0.45
1:A:404:THR:N	1:A:405:PRO:CD	2.80	0.45
1:C:590:ASP:OD2	1:C:593:THR:OG1	2.30	0.45
1:F:581:ASP:OD2	1:F:581:ASP:N	2.46	0.45
1:A:307:ARG:HD2	1:C:383:ARG:NH2	2.32	0.44
1:A:317:ALA:O	1:A:321:PHE:CD1	2.70	0.44
1:B:403:VAL:CG1	1:B:405:PRO:HD2	2.46	0.44
1:F:421:ILE:HG22	1:F:422:LEU:N	2.32	0.44
1:A:524:ASN:CG	2:A:2037:HOH:O	2.56	0.44
1:A:435:LYS:HA	1:A:460:LEU:HD13	1.98	0.44
1:F:348:GLU:HG2	1:F:379:GLU:HG2	1.99	0.44
1:A:396:THR:O	1:A:399:TYR:N	2.47	0.44
1:C:377:THR:HG23	2:C:2003:HOH:O	2.17	0.44
1:C:452:ASP:OD2	1:C:481:ARG:NH2	2.51	0.44
1:F:425:LEU:HD23	1:F:425:LEU:N	2.30	0.44
1:B:536[B]:ARG:NH1	1:B:536[B]:ARG:CG	2.75	0.44
1:B:553:ARG:HD2	1:B:558:GLU:HG2	1.99	0.44
1:C:394:ARG:HA	1:C:400:ALA:HA	1.99	0.44
1:F:468:ASP:N	1:F:468:ASP:OD1	2.51	0.44
1:A:365:ASN:C	1:A:365:ASN:OD1	2.56	0.44
1:A:529:CYS:CB	1:A:538:ALA:HB2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:ARG:O	1:B:308:ARG:C	2.57	0.43
1:B:484:ASP:OD1	1:B:486:LEU:HB3	2.18	0.43
1:A:437:LEU:O	1:A:440:ALA:HB3	2.19	0.43
1:B:519:ILE:HG21	1:B:549:GLN:NE2	2.34	0.43
1:C:298:HIS:CE1	1:C:304:GLU:HG3	2.53	0.43
1:C:377:THR:OG1	1:C:459:VAL:HG13	2.19	0.43
1:F:478:LEU:HD22	1:F:488:TRP:NE1	2.32	0.43
1:A:445:ASP:OD2	1:A:448:SER:OG	2.37	0.43
1:F:505:VAL:HG13	1:F:525:LEU:HD11	2.01	0.43
1:B:536[B]:ARG:HE	1:B:598:PHE:HD2	1.67	0.43
1:B:431:PHE:CE2	1:B:432:LEU:HD12	2.54	0.43
1:C:535:HIS:O	1:C:539:VAL:HG23	2.19	0.43
1:C:377:THR:OG1	1:C:459:VAL:CG1	2.67	0.42
1:C:470:ALA:HB3	1:C:494:THR:HG21	2.01	0.42
1:F:570:LEU:O	1:F:571:ARG:C	2.57	0.42
1:B:470:ALA:HB3	1:B:494:THR:HG21	2.00	0.42
1:A:568:SER:HA	2:A:2049:HOH:O	2.20	0.42
1:A:502:GLU:O	1:A:505:VAL:HB	2.19	0.42
1:C:364:ASP:HB3	1:C:395:TYR:CD2	2.55	0.42
1:C:478:LEU:HD22	1:C:488:TRP:NE1	2.34	0.42
1:F:431:PHE:CZ	1:F:464:SER:HB3	2.54	0.42
1:B:536[B]:ARG:NH1	1:B:536[B]:ARG:HG3	2.33	0.42
1:A:300:GLN:HE22	1:A:302:PHE:HB3	1.84	0.41
1:B:441:ALA:O	1:B:442:VAL:C	2.59	0.41
1:F:336:GLN:N	1:F:358:CYS:SG	2.93	0.41
1:C:421:ILE:HG22	1:C:422:LEU:N	2.34	0.41
1:F:503:GLU:OE1	1:F:503:GLU:N	2.51	0.41
1:A:307:ARG:O	1:A:308:ARG:C	2.58	0.41
1:A:571:ARG:CD	1:A:587:ASP:OD1	2.68	0.41
1:B:317:ALA:O	1:B:321:PHE:CD1	2.73	0.41
1:A:428:ASP:OD1	1:A:429:SER:N	2.53	0.41
1:A:314:LEU:O	1:A:315:PRO:C	2.59	0.41
1:A:554:GLY:CA	1:A:558:GLU:HB2	2.50	0.41
1:B:451:PRO:HG2	1:B:481[B]:ARG:HE	1.86	0.41
1:B:551:LYS:NZ	1:B:602:GLN:OXT	2.53	0.41
1:B:567:TRP:CE2	1:B:589:ARG:HG3	2.56	0.41
1:F:423:GLY:O	1:F:424:SER:OG	2.33	0.41
1:F:523:TYR:O	1:F:526:GLY:N	2.54	0.41
1:B:336:GLN:NE2	1:B:365:ASN:HD21	2.18	0.41
1:C:489:ASN:HB3	2:C:2007:HOH:O	2.21	0.41
1:A:572:LEU:CD2	1:A:576:MET:CE	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308:ARG:HG3	1:C:320:LEU:CD1	2.51	0.40
1:C:352:ILE:HG23	1:C:372:LEU:HD11	2.03	0.40
1:F:538:ALA:O	1:F:539:VAL:C	2.59	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	296/319 (93%)	263 (89%)	29 (10%)	4 (1%)	11 20
1	B	297/319 (93%)	276 (93%)	21 (7%)	0	100 100
1	C	299/319 (94%)	275 (92%)	18 (6%)	6 (2%)	7 12
1	F	298/319 (93%)	269 (90%)	23 (8%)	6 (2%)	7 12
All	All	1190/1276 (93%)	1083 (91%)	91 (8%)	16 (1%)	11 21

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	287	TYR
1	C	557	GLY
1	C	558	GLU
1	F	425	LEU
1	F	427	SER
1	F	558	GLU
1	C	421	ILE
1	C	423	GLY
1	F	421	ILE
1	A	558	GLU
1	C	427	SER
1	F	428	ASP

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Mol	Chain	Res	Type
1	F	429	SER
1	A	559	GLY
1	A	397	PRO
1	A	404	THR

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	248/258 (96%)	232 (94%)	16 (6%)	17	33
1	B	249/258 (96%)	232 (93%)	17 (7%)	16	30
1	C	249/258 (96%)	237 (95%)	12 (5%)	25	48
1	F	248/258 (96%)	232 (94%)	16 (6%)	17	33
All	All	994/1032 (96%)	933 (94%)	61 (6%)	18	36

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	291	GLU
1	A	292	GLU
1	A	308	ARG
1	A	310	GLN
1	A	404	THR
1	A	428	ASP
1	A	448	SER
1	A	486	LEU
1	A	515	GLN
1	A	520	ARG
1	A	552	SER
1	A	556	ARG
1	A	558	GLU
1	A	571	ARG
1	A	579	GLN
1	A	600	LEU
1	B	284	ASP

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Mol	Chain	Res	Type
1	B	291	GLU
1	B	292	GLU
1	B	303	GLU
1	B	320	LEU
1	B	367	THR
1	B	382	GLN
1	B	404	THR
1	B	428	ASP
1	B	432	LEU
1	B	500	GLN
1	B	515	GLN
1	B	520	ARG
1	B	571	ARG
1	B	579	GLN
1	B	600	LEU
1	B	602	GLN
1	C	291	GLU
1	C	292	GLU
1	C	308	ARG
1	C	431	PHE
1	C	500	GLN
1	C	515	GLN
1	C	518	TYR
1	C	520	ARG
1	C	530	ILE
1	C	571	ARG
1	C	572	LEU
1	C	579	GLN
1	F	300	GLN
1	F	310	GLN
1	F	367	THR
1	F	382	GLN
1	F	425	LEU
1	F	426	LEU
1	F	428	ASP
1	F	443	ARG
1	F	515	GLN
1	F	518	TYR
1	F	520	ARG
1	F	530	ILE
1	F	556	ARG
1	F	558	GLU

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Mol	Chain	Res	Type
1	F	571	ARG
1	F	579	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	298	HIS
1	A	336	GLN
1	A	347	GLN
1	A	366	GLN
1	A	489	ASN
1	A	524	ASN
1	B	298	HIS
1	B	326	GLN
1	B	331	HIS
1	B	336	GLN
1	C	298	HIS
1	C	336	GLN
1	C	489	ASN
1	C	524	ASN
1	F	298	HIS
1	F	336	GLN
1	F	489	ASN
1	F	524	ASN
1	F	579	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	297/319 (93%)	0.34	2 (0%)	87	89	13, 22, 26, 29	0
1	B	297/319 (93%)	0.39	5 (1%)	70	72	17, 23, 27, 31	0
1	C	302/319 (94%)	0.87	47 (15%)	2	1	20, 23, 25, 28	1 (0%)
1	F	302/319 (94%)	0.82	47 (15%)	2	1	20, 23, 25, 28	0
All	All	1198/1276 (93%)	0.61	101 (8%)	11	11	13, 23, 26, 31	1 (0%)

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	320	LEU	6.1
1	C	337	TYR	5.5
1	C	403	VAL	5.4
1	F	402	LEU	5.3
1	C	335	TRP	4.7
1	C	421	ILE	4.6
1	F	429	SER	4.5
1	F	555	PRO	4.4
1	C	301	PRO	4.3
1	C	367	THR	4.3
1	F	367	THR	4.2
1	F	330	LYS	4.1
1	C	299	PRO	4.0
1	F	426	LEU	4.0
1	C	420	ARG	4.0
1	F	298	HIS	3.9
1	C	286	GLY	3.9
1	C	294	PRO	3.9
1	C	318	VAL	3.9
1	F	309	LEU	3.8
1	F	296	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	F	337	TYR	3.7
1	C	402	LEU	3.7
1	C	444	LEU	3.7
1	F	420	ARG	3.7
1	C	425	LEU	3.6
1	C	307	ARG	3.6
1	F	421	ILE	3.5
1	C	391	ASP	3.5
1	F	312	GLY	3.4
1	C	330	LYS	3.3
1	C	309	LEU	3.3
1	C	296	ARG	3.2
1	C	555	PRO	3.2
1	C	554	GLY	3.2
1	F	289	PHE	3.2
1	F	294	PRO	3.2
1	C	356	ARG	3.2
1	F	425	LEU	3.2
1	C	556	ARG	3.2
1	C	429	SER	3.2
1	F	297	ASP	3.1
1	C	401	HIS	3.1
1	F	356	ARG	3.1
1	F	318	VAL	3.1
1	F	293	ASN	3.0
1	C	288	GLN	3.0
1	C	394	ARG	2.9
1	F	351	ALA	2.9
1	F	433	GLU	2.9
1	F	320	LEU	2.9
1	F	288	GLN	2.8
1	C	392	TRP	2.8
1	C	426	LEU	2.8
1	F	335	TRP	2.7
1	F	307	ARG	2.7
1	B	447	THR	2.7
1	F	362	LYS	2.6
1	B	404	THR	2.6
1	F	360	GLU	2.6
1	C	431	PHE	2.6
1	F	329	PRO	2.6
1	F	292	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	315	PRO	2.5
1	F	390	ARG	2.5
1	C	326	GLN	2.5
1	F	311	GLU	2.5
1	B	286	GLY	2.5
1	F	321	PHE	2.5
1	C	327	GLN	2.5
1	C	427	SER	2.5
1	C	395	TYR	2.5
1	F	306	LEU	2.4
1	F	403	VAL	2.4
1	C	558	GLU	2.4
1	A	285	LYS	2.4
1	C	291	GLU	2.4
1	C	314	LEU	2.4
1	C	302	PHE	2.3
1	C	390	ARG	2.3
1	F	302	PHE	2.3
1	F	453	VAL	2.3
1	F	371	ALA	2.3
1	F	401	HIS	2.3
1	C	359	LEU	2.3
1	C	358	CYS	2.2
1	C	376	PHE	2.2
1	B	405	PRO	2.2
1	F	322	GLU	2.2
1	F	333	GLU	2.2
1	F	440	ALA	2.2
1	F	437	LEU	2.2
1	F	295	LEU	2.2
1	C	438	PHE	2.1
1	F	438	PHE	2.1
1	C	305	GLY	2.1
1	F	299	PRO	2.1
1	A	404	THR	2.1
1	C	433	GLU	2.1
1	B	536[A]	ARG	2.1
1	F	319	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.